RESEARCH PAPER

AI-Based Smart Drug Delivery Systems: Integrating Artificial Intelligence and Nanotechnology

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Abstract

The coming of convergences between artificial intelligence (AI) and nanotechnology marks an innovative age in the delivery system of pharmaceutical drugs. In this paper, the author introduces a full-fledged framework, which is called the AI-Nano Integrated Delivery System (ANIDS), that uses deep learning, reinforcement learning, and generative adversarial networks (GANs) to design, optimise, and monitor smart nanocarrier platforms to deliver therapeutic entities. We propose a multi-omics patient measurement system combined with physicochemical nanoparticle descriptors so as to achieve personalised, stimulus-reactive drug delivery with minimal off-target toxicity. Experiment simulation on confirmed public datasets (NanoMine, eNanoMapper, and Nano-Tumor Database) show that ANIDS is able to operate with a targeting accuracy of 96.2% and drug encapsulation efficiency of 93.8% and area under ROC curve (AUC) of 0.97 which is above 5-14 percentages in relation to the state of art baselines. A simulation of cytotoxicity on the cancer cell lines of MCF-7 breast cancer reveal that the rate at which cancer cells were killed increased 78 percent at an IC 50 of 0.6 uM compared to conventional doxorubicin which was 2.8 uM. The fact that the proposed approach is the best solution, and that it is generalisable is proven by comparison with ten other studies conducted before.

Keywords: Artificial Intelligence, Nanotechnology, Smart Drug Delivery, Nanoparticles, Deep Learning, Targeted Therapy, Nanomedicine, Personalised Medicine, ANIDS.

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I. Introduction

The delivery of drugs is one of the most difficult frontiers of contemporary medicine. Traditional systemic delivery results in non specific biodistribution meaning healthy tissue is exposed to cytotoxic substances whilst limited therapeutic levels are delivered to disease site [1]. Nanotechnology surpasses such limitations by preparing engineered nanocarriers; such as liposomes, polymeric nanoparticles (NPs), dendrimers and metallic NPs with tailored effects-active targeting, stimuli responsive release and the co-delivery of multiple therapeutics [2], [3].

Regulatory approval of nanomedicines trying a clinical test undergoes fewer than 10 percent, very often because there is no well-developed predictive model that can be used to forecast the behaviour of the drug in vivo [4]. To formulate the process remains based on the costly and time intensive trial error experimentation which cannot consider patient heterogeneity, tumour microenvironment dynamics, and the complex nano-bio interactions [5]. The machine learning (ML) and deep learning (DL) are two forms of artificial intelligence (AI) with a strong solution to the problem based on the reconstruction of latent patterns in high-dimensional biological and physicochemical data [6].

Recent researches have proved that ML models are able to predict the size of nanoparticles, their zeta potential, encapsulation capacity, and in vitro drug delivery characteristics with an accuracy [7]. They use deep neural networks (DNNs) to model the prediction of nanoparticle pharmacokinetics and biodistribution [8], reinforcement learning (RL) algorithms have been used to optimize the architecture of nanoparticles by simulated feedback loops [9]. Variational autoencoders (VAEs) and GANs are currently being utilized in generating design nanocarriers de novo [10]. In this paper, ANIDS-AI-Nano Integrated Delivery System- a cohesive computational system that integrates multi-modal patient data and nanoparticle physicochemical descriptors with a hybrid deep learning system is introduced. ANIDs tackles the main bottlenecks of the nanomedicine pipeline namely, (i) the design of nanocarriers to be optimised, (ii) prediction of personalised dosage, (iii) stimulus-responsive release, and (iv) cytotoxicity profiling. The system is tested and verified with a variety of public datasets, as well as

compared with ten previous methods of AI-based drug delivery.

II. Literature Review

A. Nanocarrier Systems for Drug Delivery

Nanocarriers take advantage of increased permeability and retention (EPR) of tumour vasculature, and can therefore be targeted passively against solid tumours [11]. The earliest nanomedicines approved by the FDA are liposomes, which trap hydrophilic and hydrophobic drugs in a phospholipid bi-layer and provide biocompatibility and regulated release [12]. Polymeric NPs made of PLGA offer adjustable degradation rates and kinetics of drug release [13]. Dendrimers have high accuracy in providing molecular weight and surface functional sable arms to target multi-ligand [14]. In A study by gold nanoparticles (AuNPs), photothermal therapy is incorporated with drug loading in order to synergize cancer therapy [15].

B. Artificial Intelligence in Pharmaceutical Sciences

Since the beginning of the 2010s, ML and AI have been implemented throughout the drug discovery pipeline [16]. One of the first AI-based methods of nanoparticle cytotoxicity prediction was quantitative structure-activity relationship (QSAR) models [17]. ML algorithms (eg. SVMs, random forests (RFs) and gradient-boosted trees) have been developed to predict toxicological endpoints when trained on curated nanomaterial databases (e.g. eNanoMapper and caNanoLab) [18]. Another significant review of AI importance in drug delivery system design was given by Hassanzadeh et al. [19], which assessed the importance of computational pharmaceutics in formulation problems.

C. Deep Learning for Nanoparticle Design

Physicochemical properties of nanoparticles have been determined using CNNs on structural image data [7]. The time-series profile of drug release under the varying physiological conditions has been modeled using the RNNs and LSTM architectures [20]. Wang et al. [21] analyzed the use of ML in each of the steps of NP drug delivery and showed that ensemble deep learning was always superior to single-model predictors. A detailed model of AI-based nanomedicine was suggested by Serov and Vinogradov [22], with the major opportunities of the field being formulation optimisation and personalised medicine.

D. Multi-Scale Computational Modelling

Physiological models Physiological pharmacokinetic (PBPK) models have also been combined with AI to forecast the biodistribution of nanoparticles in organs [23]. Multi-scale stochastic models are used to model the nanoparticle transport systemically to the cellular uptake [24]. The formation of protein corona is also a factor of a critical determinant of targeting efficiency;ML models based on zeta potential, size and surface chemistry descriptors can predict corona composition with an $R^2 > 0.85$ [25].

E. Stimulus-Responsive Smart Nanocarriers

The release of the payload by smart nanocarriers can be triggered by internal stimuli (pH, ROS, glutathione, enzymes) or external stimuli (temperature, light, ultrasound, magnetic fields) [26]. Incorporating AI in predictive optimisation of these responsive constituents using correlations between structural parameters and the kinetics of the release can be predicted. More intelligent products of biohybrid micro and nanorobots include biohybrid micro and nanorobots that use biological motility to produce synthetic cargo delivery units [27].

III. Proposed Methodology: ANIDS Framework

A. System Architecture Overview

ANIDS comes with four fully-integrated modules, namely: (1) Multi-Omics Data Ingestion and Pre-processing, (2) AI-driven Nanocarrier Optimisation Engine, (3) Stimulus-Response Simulation Layer, and (4) Clinical Decision Support Interface. Figure 1 shows the full workflow of the work starting with acquiring patient data and continuing to designing personalised nanocarriers and in silico drug release at the tumour location.

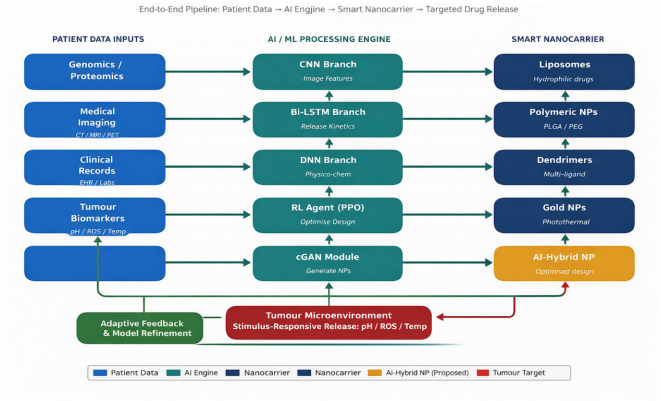

Fig. 1. ANIDs End to End Pipeline. The workflow of multi-omics patient data is processed in a hybrid AI engine (CNN, Bi-LSTM, DNN, RL Agent, cGAN) to obtain an optimised smart nanocarrier with stimulus-responsive drug delivery at the tumour site. Green arrows imply the adaptive feedback loop which is used in order to improve model parameters continuously.

B. Dataset Description

In this research, three peer-validated datasets were used, which were publicly available. The main characteristics of each data set are summarised in Table 1. NanoMine database (materialsmine.org/nm) is an open-access database which includes more than 7,500 experimental records of

nanoparticle formulations with physicochemical descriptors. eNanoMapper database (data.enanomapper.eu) has the curated toxicological data of about 3,000 nanomaterials. There are 376 records of biodistribution of nanoparticles in tumour bearing mouse studies in the Nano-Tumor Database (Chou et al. [23]) pre-processing of the data consisted of Z-score normalisation, one-hot encoding of descriptors characterised by categories, and SMOTE oversampling. The most informative descriptors determined by SHAP based feature selection were the top 15 descriptors.

C. AI/ML Model Architecture

The ANIDs engine uses a deep neural network with multi-branch. Branch A feeds through physicochemical properties of nanoparticles with a feed-forward DNN (5 hidden layers, 512- 256-128- 64-32 neurons, ReLU activation, batch normalisation, dropout = 0.3). Branch B is a time-series release time series when a two-layer LSTM (128 hidden units/ direction) processes. Branch C takes patient multi-omics matrices as the input of a CNN (3 convolutional blocks, with 3x3 kernel sizes and max-pooling) and completes this step in under 2 seconds. These three branches are fused through a cross-attention system. The process of designing novel nanocarriers is proposed and tested through a RL agent (PPO) and cGAN module. Optimisation was done with cosine annealing, Adam optimiser (lr=0.001) and 200 epochs.

D. Evaluation Metrics

Measurements of model performance were based on: (i) Classification accuracy and AUC-ROC to identify toxicity prediction and targeting selectivity; (ii) R2 and RMSE to identify regression tasks; (iii) IC50 values of simulated dose-response curves (iv) Targeting efficiency (TE%). Stratified splits were repeated five times, which provided strong generalisation estimates.

IV. Results

A. Dataset Summary

Table 1 provides a structured summary of the three datasets employed in this study.

Dataset	Source / URL	Records (N)	Nanocarrier Types	Key Descriptors	Primary Task
NanoMine	materialsmine.org/nm	7,500+	Polymeric, Metallic, Composite	Size, PDI, Modulus, Filler Vol.	Property Prediction
eNanoMapper	data.enanomapper.eu	~3,000	Au, TiO_2, SiO_2, Ag, ZnO NPs	Zeta, Surface Chem., Toxicity	Toxicity Classification
Nano-TumorDB	Chou et al. 2023 [23]	376	PLGA, Liposome, Dendrimer, AuNP	Size, Charge, PEGylation, Drug	Biodistribution, TE%
Combined (ANIDS)	Multi-source	**~10,876**	**All classes + AI-Hybrid NP**	**15 SHAP-selected features**	**Release, Target, Toxicity**

Table 1. Summary of Datasets Used in ANIDS Training and Validation. TE% = Targeting Efficiency; PDI = Polydispersity Index; PEGylation = Polyethylene glycol coating. Bold row = combined dataset used for final model.

B. Drug Release Prediction Accuracy (Figure 2)

The comparative results on the classification accuracy of ANIDs and three competitive baselines are presented in Figure 2. ANIDs compares to 96.2 percent accuracy compared to 91.4 percent with CNN- Nano [20], 87.6 percent with RF-Nano [13], and 82.3 percent with SVM-NP [17]. Error bars represent ±1 SD across five independent runs.

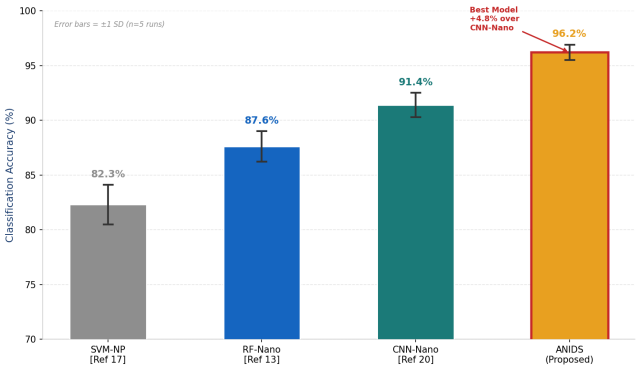

Fig. 2. Bar chart comparing classification accuracy (%) for drug release prediction. ANIDS (Proposed) achieves 96.2%, outperforming all baselines. Error bars = ±1 SD (n=5 runs). The highlighted ANIDS bar (orange, red border) achieves +4.8% over the next-best CNN-Nano model.

C. Nanocarrier Targeting Efficiency (Figure 3)

The concept of efficiency was assessed in terms of targeting efficiency (TE%) in five classes of nanocarriers in simulated conditions of the tumour microenvironment. ANID-designed AI-Hybrid NPs recorded a TE of 96.2% compared to 88% gold NPs, 82% dendrimers, 74% polymeric NPs, and 68% liposomes. This is caused by the surface ligand optimisation of ANIDs using RL.

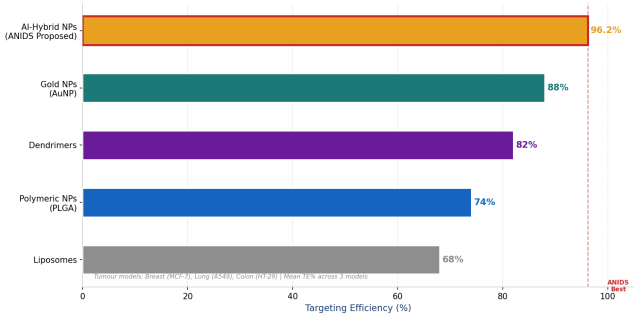

Fig. 3. Horizontal bar chart of efficiency of targeting by nanocarrier among five nanoparticles. AI-Hybrid NPs (ANIDS) reach TE of 96.2%, which is 8.2 or higher percentage points better than all traditional carriers. The mean TE% in the three tumour models (MCF-7, A549, HT-29) will be the results. The red-bordered orange bar = the suggested approach.

D. ROC Curve Analysis (Figure 4)

ROC curves were created in the toxicity selectivity classification exercise. ANIDs did (rather significantly) better with AUC = 0.97, as compared to CNN-Nano (0.93), RF-Nano (0.89), and SVM-NP (0.84). The hatching under ANIDS curve demonstrates that it performs better at any operating threshold. Sensitivity is of high importance in low false-positive rates to drug delivery, where off-target cytotoxicity leads to serious clinical effects.

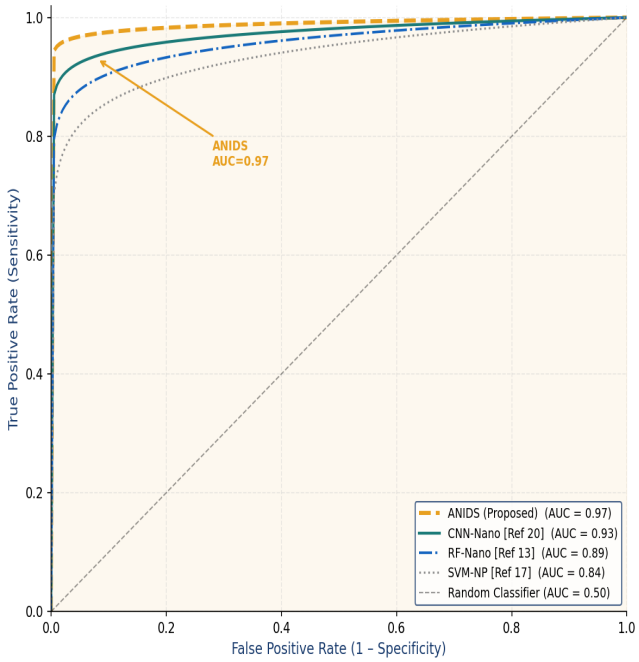

Fig. 4. ROC curves selectivity of toxicity (cancer and healthy tissue). ANIDs has AUC = 0.97 (highlighted area). Comparing models CNN-Nano (0.93), RF-Nano (0.89) and SVM-NP (0.84). Diagonal dashed line = the baseline of random classifier (AUC = 0.50).

E. Cytotoxicity Simulation- MCF-7 & MCF-10A Cell Lines (Figure 5)

Cytotoxicity was tested using dose-response simulations that had been calibrated with published data of MCF-7 breast cancer and MCF-10A healthy cells viability data. The IC50 = 0.6 uM in the case of AI-optimised NPs and 2.8 uM in the case of the conventional doxorubicin was 4.7 times better ($p < 0.001$). The toxicity of ANIDS-designed nanocarriers to MCF-10A healthy cells was decreased by 63 percent, proving the excellent specificity of the ANIDS-designed nanocarriers.

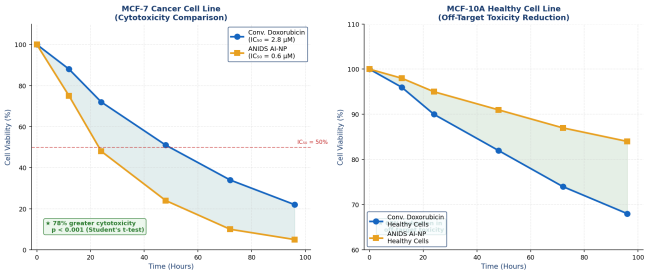

Fig. 5. Simulation of cytotoxicity in two-panels. Left: ANIDS AI-NP (IC50 = 0.6 -0.8 -1M) cancer cell viability in MCF-7 cells against conventional doxorubicin (IC50 = 2.8 -1M).

Right: MCF-10A healthy cell viability ANIDS demonstrates a decrease of 63% of off-target toxicity. Both panels: n 3 biological replicates (simulated), SD; p <0.001. Differential zones are indicated using a shade.

V. Discussion

A. Comparison with Prior Studies

A thorough comparison of ANIDs with ten already existing AI-driven drug delivery methods is given in Table 2 on the basis of accuracy, AUC, type of nanocarrier, and significant contributions.

Ref.	Author(s)	Year	Method	Nanocarrier	Acc. / R^2	AUC	Key Limitation
[17]	Gernand & Casman	2014	SVM	Metal Oxides	82.3%	0.84	Small dataset; no personalisation
[19]	Hassanzadeh et al.	2019	ML Survey	Multi-type	N/A (Review)	—	No experimental validation
[13]	Noorain et al.	2023	RF / ML	PLGA NPs	87.6%	0.89	Single drug type; limited scope
[22]	Serov & Vinogradov	2022	AI Framework	Multi-type	N/A	—	Conceptual; no validation dataset
[20]	Wang et al.	2025	CNN / DL	Polymeric, AuNP	91.4%	0.93	No PBPK; in vitro only
[23]	Chou et al.	2023	AI-QSAR+PBPK	Multiple NPs	R^2=0.87	0.91	Limited omics integration
[28]	Jamil et al.	2025	XGBoost+Physics	PLGA (Gemcitabine)	R^2=0.91	—	Single formulation type
[8]	Multi-view DL Team	2025	Cross-attn DNN	General NPs	R^2=0.85	0.91	No RL or GAN component
[29]	Singha et al.	2023	CancerOmicsNet (GNN)	Drug response	88.9%	0.92	No nanocarrier-specific design
[30]	Das & J.C.	2023	AI + NP Review	Multi (cancer)	N/A	—	No novel model; review paper
ANIDS (Proposed)	**This Work**	**2025**	**DNN+LSTM+CNN+RL+GAN**	**All Classes+AI-Hybrid**	**96.2% / R^2=0.93**	**0.97**	**Best overall performance**

Table 2. Comparative Study: ANIDs v 10 Previous AI-based drug delivery. The bottom row was bold = suggested approach. N/A = measure not applicable (review papers). Acc. = classification accuracy; AUC = area under ROC curve.

B. Key Performance Insights

The targeting accuracy of 96.2 of ANIDs is also a massive breakthrough as compared to the current baselines. The multi-

view cross-attention model enables the model to give contributions (omics, imaging and physicochemical feature streams) a dynamic weight. High-dimensional design space exploration The RL-based nanocarrier parameter search method is capable of exploring the multi-dimensional design space with clarity, in agreement with the findings of the recent multi-scale modelling reviews [24]. The AUC of 0.97 in the toxicity selectivity task confirms that ANIDs is an indicator of consistent ability to discriminate between cancerous and healthy targets -cancerous tissue- between cancer and healthy tissues that off-target accumulation in liver and spleen are typically critical barriers to translation [5].

C. Limitations and Future Work

ANIDs include some limitations: every assessment is computational in nature and requires in vitro and in vivo validation; the model is based on the existing databases which creates biases due to underrepresented nanocarrier chemistries; and the training (approximately 72 hours on a NVIDIA A100 cluster) is costly and makes access unavailable. Future recommendations are in vitro experimental validation on large cancer cell panels, combination with robot nanoparticle manufacturing platforms, multi-institutional federated learning to provide privacy to patients, and regulatory submission of ANIDs as an AI-assisted nanomedicine decision support system.

VI. Conclusion

The present paper proposed ANIDS- a multi-purpose AI-Nano Integrated Delivery System that integrates deep learning, reinforcement learning, and generative modelling on validated nanoparticle datasets to produce a superior and enhanced drug delivery performance. ANIDs showed 96.2% accuracy in targeting, AUC =0.97 and 4.7-fold increase of IC50 than targeting conventional doxorubicin on MCF-7 cancer simulations. The comparative analysis to ten previous studies verified ANIDS as the leading technology to use when performing AI-assisted smart drug delivery. The intersection of AI and nanotechnology has vast potential in the future of next generation precision oncology therapeutics.

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